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NEAREST NEIGHBOR SPACINGS OF CLEAN VANADIUM SURFACES FROM EXTEN--ETC(U)
JUN 78 W T ELAM, P I COHEN, L ROELOFS N00014-75-C-0292

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(6) NEAREST NEIGHBOR SPACINGS OF CLEAN VANADIUM SURFACES FROM EXTENDED APPEARANCE POTENTIAL FINE STRUCTURE

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Fine structure in the excitation probability of the 2p core state of vanadium by electron bombardment has been found to extend for several hundred volts above the appearance potential threshold. The structure results from interference of an outgoing spherical wave of a scattered electron with backscattered components from neighboring atoms. It is therefore analogous to extended X-ray absorption fine structure (EXAFS) and it should be possible to extract geometric information using the same Fourier inversion techniques. The short mean free path for inelastic scattering of the incident electrons, however, renders the technique sensitive to the structure in just the outermost layers of the material.

Initial attempts at Fourier inversion of the extended appearance potential fine structure of vanadium met with little success.[1] Several complications that might account for this failure were considered, including the lack of dipole selection rules, and the effect of multiple scattering. We have since learned, however, that failure to adequately take account of background variations was the principal difficulty. Once these variations are sufficiently reduced, Fourier inversion of the spectrum as a function of k yields an atomic spacing consistent with the known nearest-neighbor spacing of bulk vanadium. Although multiple scattering and other complications are presumably still important,[2] they do not preclude the extraction of atomic spacings from extended appearance potential fine structure (EAPFS).

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The background is evident in the portion of the second-derivative 2p appearance potential spectrum of a clean vanadium surface shown in Fig. 1. This structure was previously identified with the 2s core level,[1] but it can be shown that extended fine structure associated with the 2s appearance potential feature is too weak to show up on this scale. The technique used to remove this background employs a least squares fit of the data to a third order polynomial. The values of this polynomial are then subtracted point by point from the data. The result is shown in Fig. 2. The zero energy of the fine structure was taken to be the $2p_{3/2}$ threshold. The first 130eV of the spectrum were omitted to suppress the effect of multiple scattering. The data extends to 570eV above the edge.

The Fourier transform of the spectrum after subtraction (Fig. 3) exhibits a prominent peak at 2.4 Å. To this value must be added approximately 0.3 Å to correct for the k-dependent backscattering phase shift,[3] giving a result of 2.7 Å, in agreement with the nearest-neighbor bulk spacing in vanadium of 2.69 Å. A smaller peak at an unphysically small distance is evidence that the background subtraction is still imperfect. The expected locations of peaks corresponding to more distant neighbors are indicated on the figure, but nothing can be concluded about these spacings at this stage of development.

The principal difficulty is the width of features in the transform. There are several factors that probably contribute to this width. Foremost, of course, is the somewhat limited range of our data. There is, however, no fundamental obstacle to increasing this range. Another important factor is that each of the various partial waves contributing to the scattering may have different phase shifts. There is, in addition, the problem of multiple edges. We have tacitly assumed in this analysis that the structure results entirely from the $2p_{3/2}$

excitation. In fact, of course, fine structure of just half the intensity, but displaced by the spin orbit splitting (7.4 eV[4]), must result from the $2p_{1/2}$ excitation. Still weaker structure due to the 2s excitation, displaced by 113.2 eV[4], must also be present. A more careful analysis must consider correlations at these displacements. Moreoever, the consequences of multiple scattering have not been assessed. We do know that if the transform includes all of the spectrum above the $2p_{3/2}$ edge, the nearest-neighbor separation is obscurred by spurious peaks in the transform, presumably resulting from multiple scattering.

We conclude that geometric information concerning the surface region of solids can be extracted from extended appearance potential fine structure by Fourier transform techniques. The use of electron excitation opens up extended fine structure analysis of surfaces to every laboratory with an ultra high vacuum system. More work is needed to define the factors limiting this approach.

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FIGURE CAPTIONS

FIGURE 1. Extended fine structure in the range 130 eV to 570 eV above the vanadium $2p_{3/2}$ core appearance potential edge (located at 508 volts on this scale). The spectrum was taken by measuring the second derivative of the sample current as a function of the incident electron accelerating potential. The apparatus is described in Ref. 1.

FIGURE 2. Vanadium extended fine structure after background removal by polynomial subtraction. The third order polynomial is found by a least squares fit to all of the data points. Note that with the background removed the periodic portion of the data is enhanced.

FIGURE 3. Magnitude of the Fourier transform of the vanadium extended fine structure after background suppression. The arrows are the expected peak positions corresponding to atomic separations in bulk vanadium after a correction of -0.3 Å for the k-dependence of the backscattering phase shift. The nearest neighbor peak is in excellent agreement. The unphysical peak at about 1.2 Å is evidence that the background is not entirely removed.

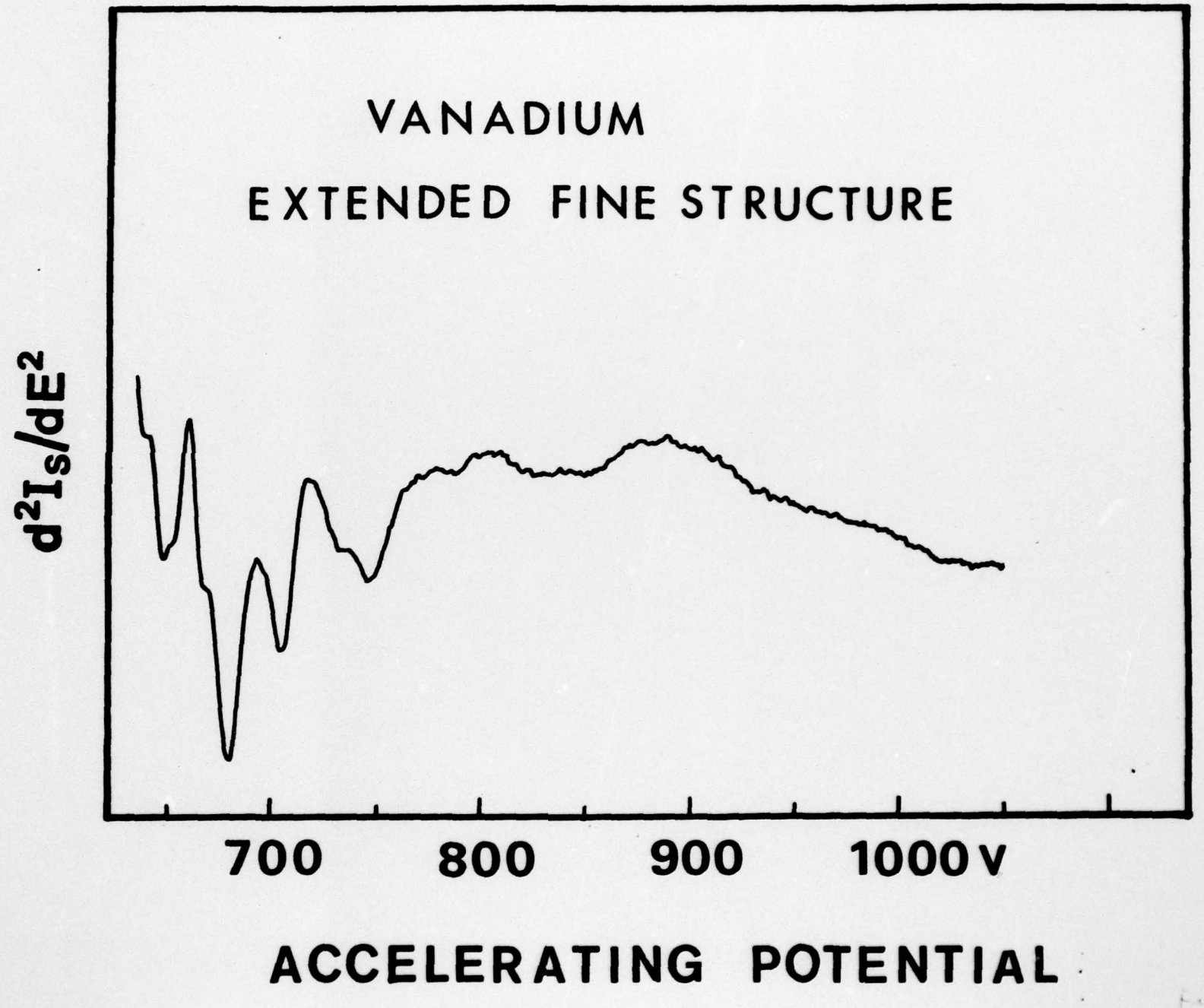
VANADIUM
EXTENDED FINE STRUCTURE
d^2I_s/dE^2
700
800
900
1000 v
ACCELERATING POTENTIAL

Fig 1

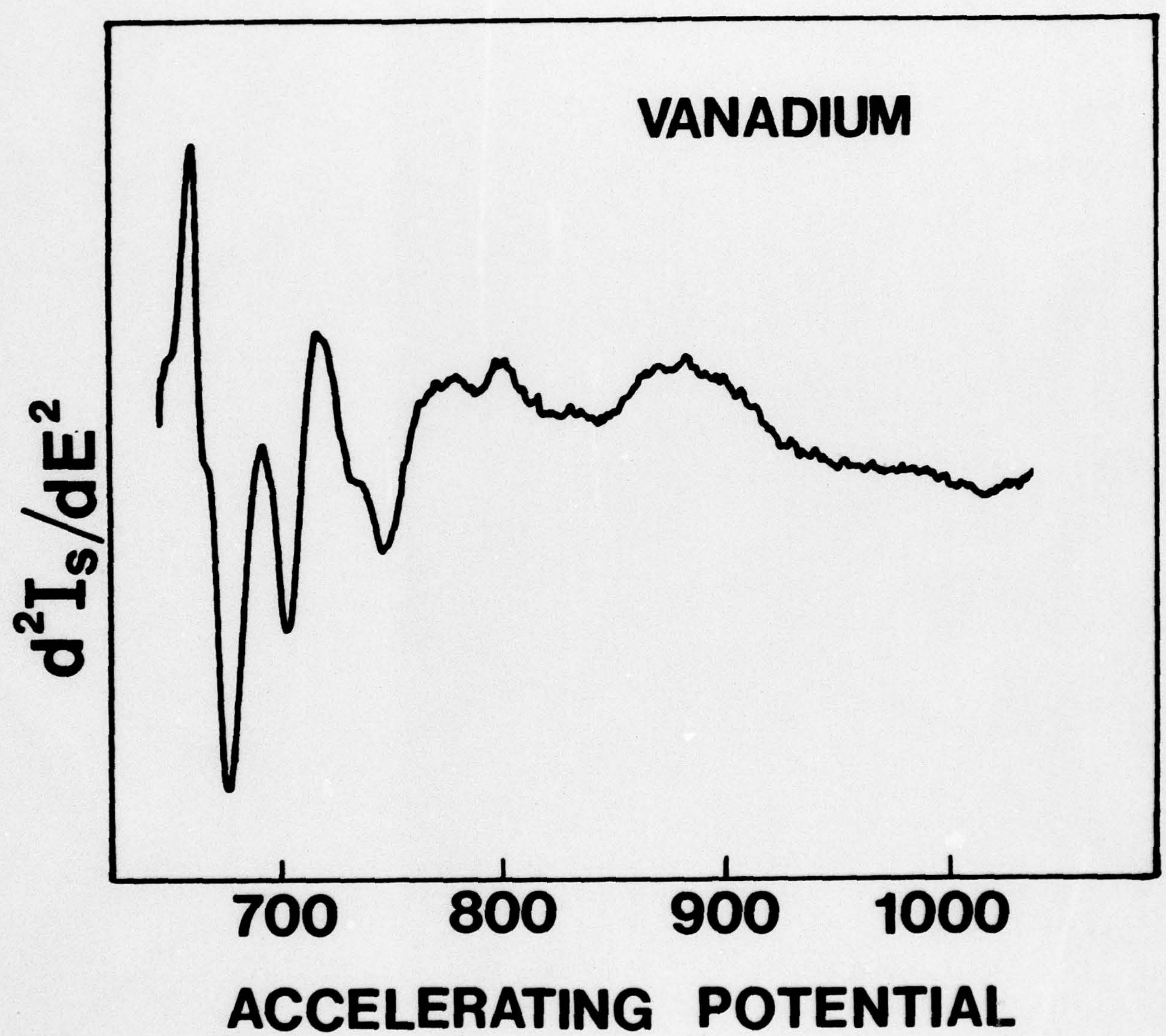

Fig. 2

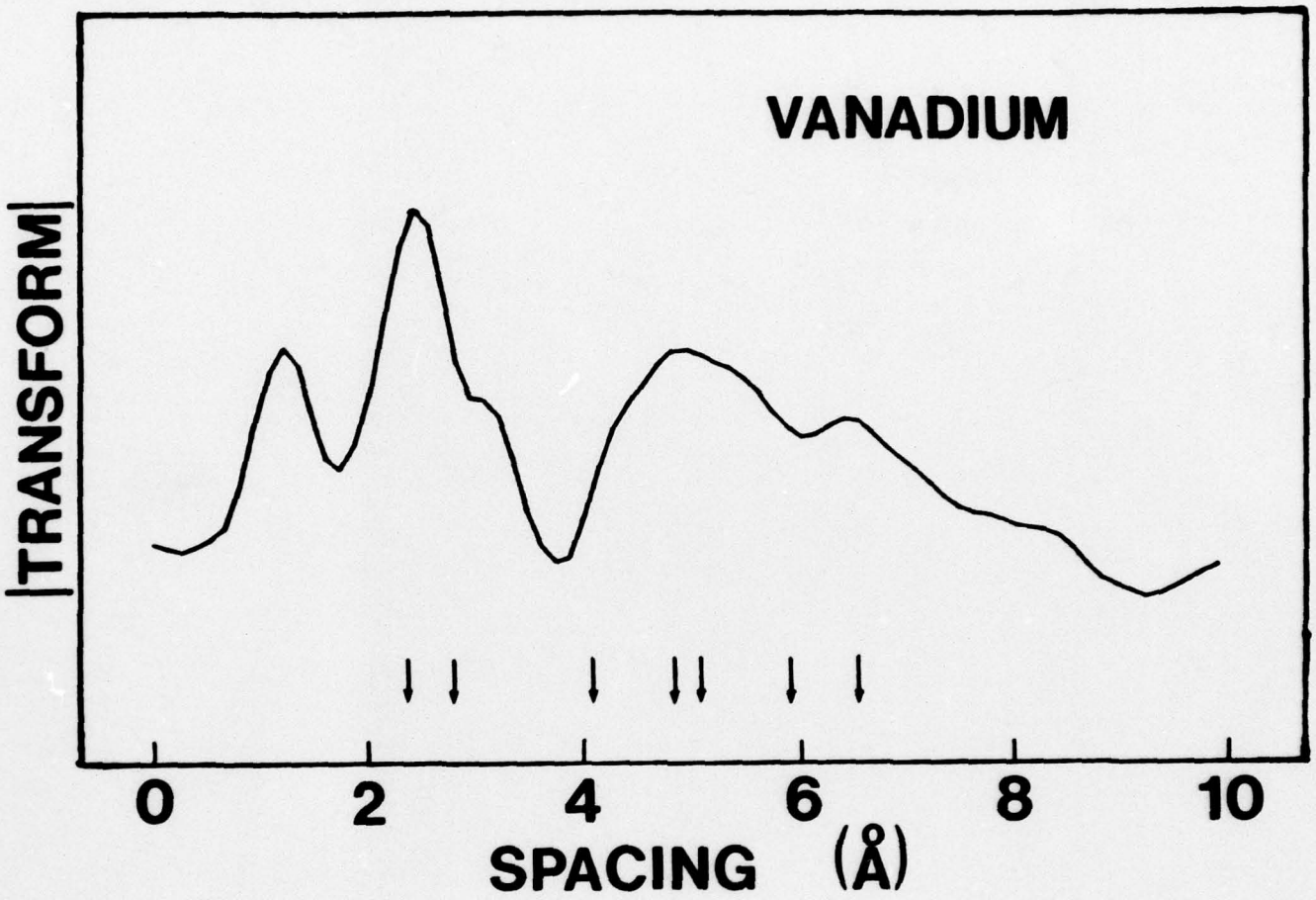

Fig. 3